IUCLID 5
Guidance and Support

Installation Guide for IUCLID 5.4
Client-Server Architecture

Linux

July 2012

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Chapter 1. Introduction

IUCLID 5 has two different installation architectures:

- Standalone installation

  The IUCLID 5 application connects directly to the database which usually resides on the same computer. Using this installation only one user can work simultaneously on the same database.

- Distributed installation

  In this architecture, the database and the application server reside on a server computer, and the user works with another computer, called a client. It is similar to a web based application with the only difference being that the user interface of the application (buttons, text boxes etc.) is not a series of web pages but a specific Java application called *IUCLID 5 client* that is downloaded automatically from the server.

This document describes how to download, install and configure the necessary open source software products and the IUCLID 5 application itself on a Linux server. Only the distributed installation is described.

The aim of this document is that a user with basic computer skills would be able to install and run IUCLID 5. The following is a list of items NOT covered in this document:

- Complete and detailed installation and configuration procedure of the operating system (GNU/Linux).
- A detailed configuration of the Database Management System (PostgreSQL) and the Application Server (Tomcat)

If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting the ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

1.1. Hardware requirements

The server hosting IUCLID 5 must have at least:

- RAM: 2 GB
- Hard disk space: 200 GB
- CPU: 2 GHz, 32 or 64 bit architecture
- Network adapter 100 Mbps (recommended 1Gbps)

The requirements depend in part on the plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database.

1.2. Software requirements

The software prerequisites for the installation are as follows:

- Java Runtime Environment (JRE) or Java Software Development Kit (SDK) 6

Note

This is not the most recent version of Java.

- PostgreSQL 8.2, 8.3, 8.4 or 9.0 (recommended).
- Tomcat 5.5 or 6.0
- The IUCLID 5 manual workstation installation package, version 5.4, can be downloaded without charge from the IUCLID 5 web site.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to at least a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID 5 web site where the installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory. These are also available from the web site at which the IUCLID 5 software is published.

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set,* a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

For more information regarding system requirements, see the FAQ on the IUCLID web site located at http://iuclid.eu.

Chapter 2. Making a fresh installation of IUCLID 5

The following chapter contains a brief description of the actions required to make a fresh installation of IUCLID 5 that runs within a web server on a Linux operating system in combination with open source components.

2.1. Operating system

You are free to run IUCLID 5 on the Linux distribution of your choice. However, only the SUSE Linux distribution has been explicitly tested. Keep in mind that it is good practice to install only the required software on a server. The file paths shown in this document are provided as examples, and as such, may differ from the values required in the actual installation.

2.1.1. Opening the network port for IUCLID 5 server

In order of establish the connection from the workstation computer to the server, the server's firewall must be configured to allow the IUCLID 5 server to accept connections on port 8080.

It is not recommended to completely disable the firewall. In CentOS for example the `system-config-securitylevel-tui` tool allows you to easily modify the firewall settings. On other Linux distributions please refer to the documentation of the operating system.

```
~#system-config-securitylevel-tui
```

Be cautious! You should not trust any network interface. In the *Allow incoming* section set SSH (secure shell) and 8080 port. For security reasons do not allow any other traffic such as telnet, http or ftp.

Before you start the installation procedure you have to download the required components for IUCLID 5. In order to select the correct files, you should know the architecture (platform) of your server computer. Please consult the user manual of your computer. If the Linux operating system is already installed, write the following command. The command will write the platform's name on the screen, for example `i386`.

```
~#uname -i
i386
~#
```

2.2. JAVA Development Kit

The simplest way to install Java is using the package manager of your operating system. In this way you do not need to download Java manually.

In case no appropriate Java runtime environment is available in the package manager, download the JAVA Development Kit (JDK) 6 or JAVA Runtime Environment (JRE) 6 according to the operating system distribution and architecture of your computer from the site http://www.oracle.com.

For example for a 32 bit computer download the `i586` version.

```
jdk-6u11-linux-i586.bin
```

If you have a computer with 64 bit processor(s) and the 64 bit version of Linux installed on it then download the 64 bit Java SDK or JRE.

```
jre-6u11-linux-x64.bin
```

If you selected Java in the package manager, it should be installed already. Otherwise run the installer.

Make the JDK file executable and start it.

```
iuclid5#chmod +x jdk-6u11-linux-i586.bin
iuclid5#./jdk-6u11-linux-i586.bin
```

The Sun binary code License Agreement prompt is displayed. Press the enter button to scroll down to the end. You are asked to accept the license. Answer *yes*.

```
Do you agree to the above license terms? [yes or no]
yes
```

Status messages are displayed as the installation proceeds. Warning messages can be ignored. After the installation check the Java environment by displaying the version.

```
iuclid5#java -version
java version "1.6.0"
Java(TM) SE Runtime Environment (build 1.6.0-b105)
Java HotSpot(TM) Server VM (build 1.6.0-b105, mixed mode)
```

For more information please consult the Java SE 6 Platform installation instructions at the site http://www.oracle.com.

2.3. PostgreSQL

PostgreSQL is the database management system (DBMS) that IUCLID 5 uses to store all data.

PostgreSQL is likely to be included in your Linux distribution. If PostgreSQL is not already installed, it is recommended to install the latest version using the package management system of your Linux distribution. Alternatively, the installation packages are available free of charge from the following site http://www.postgresql.org.

You do not need to download all the installation packages. The required packages have a file name that starts with `postgresql-libs-`, `postgresql-server` or `postgresql`.

2.3.1. Creating the iuclid5 database user

During installation process, a new Linux user with name *postgres* is created. The user *postgres* has no password, so it is not possible to log in using this user name. Its purpose is to perform database administrative tasks. Commands can be run as user `postgres`, only using the command *su*.

Change the current directory and the current user, as follows.

```
$cd /
$su postgres
$
```

Note

By changing the user, the prompt is also changed to the $ sign (and usually *bash-3.00$* is displayed).

Now each command you type is executed as the user *postgres*. The first thing to do is to create a database user that allows the IUCLID 5 application to connect to the database, as shown below. The name of the user is usually

iuclid5. Enter a password, enter it again, and then answer "no" to all the subsequent questions. To answer "no", enter "n", and then press the *enter* key.

Note

Remember the password you give for the user *iuclid5*, because you will need it later.

```
$createuser -EP iuclid5
Enter password for new role:
Enter it again:
Shall the new role be a superuser? (y/n) n
Shall the new role be allowed to create databases? (y/n) n
Shall the new role be allowed to create more new roles? (y/n) n
CREATE ROLE
$
```

2.3.2. Creating the iuclid5 database

Create a new database specifying the owner, encoding and the name of the database.

```
$createdb --owner=iuclid5 --encoding=UTF-8 iuclid5
CREATE DATABASE
$
```

Once the database preparation tasks are completed, change back to the root user.

```
$exit
/#
```

For security reasons, by default, database users are not allowed to connect to the database, even if they provide the correct password. However, PostgreSQL can be configured to allow such a connection, as described below.

Open the configuration file using a text editor, for example **nano**.

```
iuclid5#nano /var/lib/pgsql/data/pg_hba.conf
# PostgreSQL Client Authentication Configuration File
# ===================================================
#
```

Move the cursor to the end of the file using the down arrow button until the line *# IPv4 local connections:*.

```
# IPv4 local connections:
host    all         all         127.0.0.1/32          ident sameuser
```

Insert a new line just after the *IPv4 local connections* and type *host iuclid5 iuclid5 127.0.0.1/32 md5*. This line tells PostgreSQL that iuclid5 user is allowed to connect to iuclid5 database from the local computer using the encrypted password authentication.

```
# IPv4 local connections:
host    iuclid5     iuclid5     127.0.0.1/32          md5
host    all         all         127.0.0.1/32          ident sameuser
```

Press CONTROL-X to exit from the editor, type *y* to save the file and confirm the file name by pressing the enter key.

```
Save modified buffer (ANSWERING "No" WILL DESTROY CHANGES) ? y
 Y Yes
 N No           ^C Cancel
```

```
File Name to Write: /var/lib/pgsql/data/pg_hba.conf
^G Get Help         M-D DOS Format      M-A Append          M-B Backup File
^T To Files         M-O Mac Format      M-P Prepend         ^C Cancel
```

Restart PostgreSQL to load the new configuration.

Your iuclid5 database is now ready to serve the IUCLID 5 application.

For more information about installing PostgreSQL and administer the server look for the http://www.postgresql.org/docs/ documentation page.

2.3.3. Set up daily backup of the database

The data you store into IUCLID 5 might be very important for your organisation. A user may accidentally delete valuable data or a system failure could cause loss of data. To prevent this situation and prepare a smooth recovery, it is vital to schedule a daily backup.

2.4. Tomcat

The preferred way to install Tomcat is by using the package manager of your operating system. The required version is 5.5.x or 6.0.x where x is the highest available number.

2.4.1. Manual installation

Distribution independent packages can be downloaded from the Tomcat website [http://tomcat.apache.org/].

The file to download is for example:

```
apache-tomcat-5.5.26.tar.gz
```

The installation of Tomcat is extracting a set of files and setting up the starting parameters. Extract the downloaded archive into the directory `/opt` (use the version number of your downloaded Tomcat).

```
iuclid5#tar -xzf apache-tomcat-5.5.26.tar.gz -C /opt
iuclid5#
```

It is convenient to create a version independent symbolic link pointing to the actual tomcat directory. It will be used to find the location of Tomcat, whichever version is installed.

```
iuclid5#ln -s apache-tomcat-5.5.26 /opt/apache-tomcat
iuclid5#
```

Tip

Tomcat contains some example applications that are not needed. You can delete them in order to save resources. Do not delete the `ROOT` directory!

For more information visit the Tomcat website [http://tomcat.apache.org/].

2.4.2. Memory settings

Important

IUCLID 5 requires at least 512 MB RAM to be allocated to Tomcat.

Check the amount of memory allocated on the server status page of the Tomcat Manager application. The parameter `Max Memory` under JVM should show a value of at least 512 MB.

Tomcat Manager

Tomcat Manager is a web application, supplied along with Tomcat, that provides a means of dynamically managing web applications without having to shutdown the Tomcat web application server itself. It provides a convenient way of managing the IUCLID 5 web application in a distributed environment. To gain access to Tomcat Manager, point a web browser to the address http://localhost:8080/manager/html/.

2.5. Deployment

Deployment is the term used for the process of installing a web application into a web application server.

The web application of IUCLID 5 is published in the form of a web application archive (WAR) which is a file with extension `war`. It is available from the IUCLID website [http://iuclid.eu/], packaged into a file named `iuclid5<version>_server_<date>.zip`. Download the ZIP file from the web site. Unzip it, and then unzip an archive within it named `server.zip`. Inside there is a file named `i5server.war`. That is the file to be deployed.

2.5.1. Deployment in Tomcat

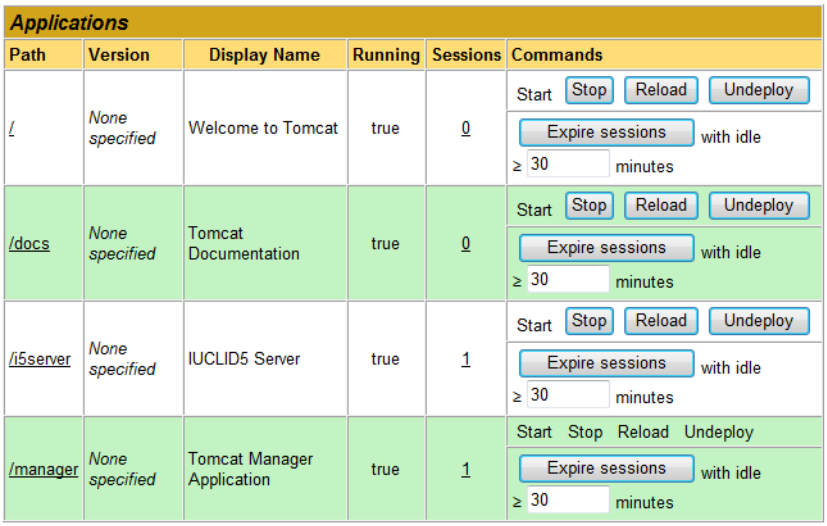
Deployment of a web application into Tomcat can be done in two ways:

- Statically - the web application is set up whilst the web application server Tomcat is not running.
- Dynamically - one or more web applications can be managed whilst the web application server Tomcat is still running. This allows IUCLID 5 to be installed on an instance of Tomcat without needing to have a break in service for any other web applications that are running on the same instance of Tomcat.

In this installation manual, only the dynamic deployment is described. However, the static deployment may be used instead. The deployment of a web application on Tomcat is described in detail on the web page Tomcat deployment [http://tomcat.apache.org/tomcat-5.5-doc/deployer-howto.html]. In essence, the deployment of IUCLID 5 consists of copying the archive file `i5server.war` into a folder within the installation of Tomcat, named `webapps`. If Tomcat is running whilst the copying is done, it automatically opens the archive and copies the content into the folder `webapps`. In addition, Tomcat automatically starts the IUCLID 5 web application.

When IUCLID 5 is deployed in Tomcat, it is shown in the list of web applications in Tomcat Manager, as shown below. If you are unfamiliar with Tomcat Manager, see the tip above.

Figure 2.1. IUCLID 5 deployed in Tomcat - application list in Tomcat Manager



Applications

Path	Version	Display Name	Running	Sessions	Commands
/	*None specified*	Welcome to Tomcat	true	0	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/docs	*None specified*	Tomcat Documentation	true	0	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/i5server	*None specified*	IUCLID5 Server	true	1	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes
/manager	*None specified*	Tomcat Manager Application	true	1	Start Stop Reload Undeploy Expire sessions with idle ≥ 30 minutes

Alternatively, deployment can be done using the deploy feature of the Tomcat Manager to upload a war file into Tomcat from a filesystem. However, before doing that, the configuration of Tomcat Manager should be checked and possibly adjusted for the following reason.

Warning

By default, Tomcat Manager places an upper limit on the size of the war file that can be uploaded. The default value of the limit is smaller than the size of the file `iuclid.war`. If the size limit is exceeded, the following error is given:

The server encountered an internal error () that prevented it from fulfilling this request. Exception java.lang.IllegalStateException: org.apache.tomcat.util.http.fileupload.FileUploadBase$SizeLimitExceededException: the request was rejected because its size (XXX) exceeds the configured maximum (52428800)

The solution is to increase the size of the limit, by increasing the values of the parameters *max-file-size* and *max-request-size* in the settings file `/tomcat7/webapps/manager/WEB-INF/web.xml` to values that are larger than that they exceed the size of the war file. The default values are shown below:

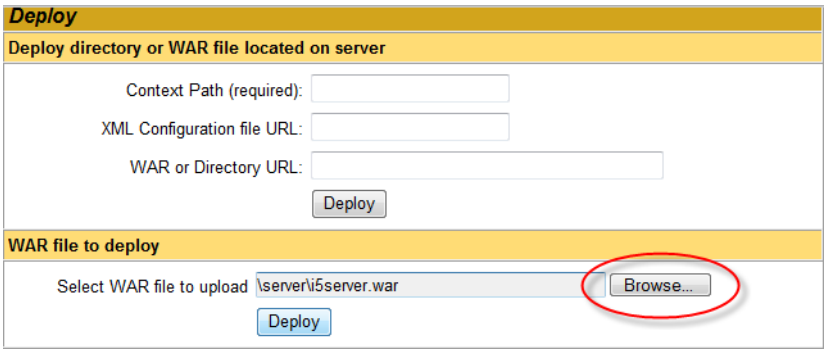
```
<multipart-config>
<!- 50MB max ->
<max-file-size>52428800</max-file-size>
<max-request-size>52428800</max-request-size>
<file-size-threshold>0</file-size-threshold>
</multipart-config>
```

An example of the new values required, for IUCLID 5.4.0, is shown below.

```
<max-file-size>80000000</max-file-size>
<max-request-size>80000000</max-request-size>
```

Once you are sure that the file size limit is large enough, in Tomcat Manager, click on the button Browse, that is under the lower of the two options deploy options, WAR file to deploy, as shown below:

Figure 2.2. Deploy IUCLID 5 in Tomcat - upload using Tomcat Manager



Browse to the file `i5server.war`, select it, and then click the button Open. Click on the lower of the buttons labelled Deploy. Check that IUCLID 5 appears within the list of web applications.

Tomcat Manager can be used to stop and start the IUCLID 5 web application. On the application list page, there are stop and start buttons for each web application currently deployed. This feature is useful for carrying out any maintenance that must be done whilst IUCLID 5 is stopped. An example is the editing of settings for the connection to the database.

2.6. Configuring the connection to the database

The configuration of the connection from the IUCLID web application to its database is defined in the file `server.properties` that is located in the folder `webapps/i5server/WEB-INF/classes`.

The default values are for an instance of the PostgreSQL database running on the same computer as the web application server with the values of the database name, the database username, and the password of that user all set to *iuclid5*. If that configuration is used, on starting the IUCLID 5 web application, it will connect to the database without the need to make any changes to the configuration file. If other values are required, they must be entered into the file `server.properties`. Before editing the configuration file, ensure that no clients are connected to the IUCLID 5 web application and then stop the application using Tomcat Manager.

The default configuration for PostgreSQL is shown below:

```
#
# Settings for using PostgreSQL
#
hibernate.connection.url=jdbc:postgresql://localhost:5432/iuclid5
hibernate.connection.username=iuclid5
hibernate.connection.password=iuclid5
hibernate.connection.driver_class=org.postgresql.Driver
hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect
```

For example, if the PostgreSQL database server's name is *dbserver*, it is accepting connections on port *12345*, the database name is *chemdb* with a database user named *joe* with a password *xxxx*, the configuration is:

```
hibernate.connection.url=jdbc:postgresql://dbserver:12345/chemdb
hibernate.connection.username=joe
hibernate.connection.password=xxxx
```

Important

Make sure that there are no spaces after the username and password values in the properties file.

After editing the configuration file, start the IUCLID 5 web application server using Tomcat Manager.

The IUCLID 5 server records its activities in a log file. The configuration file for the logging is `i5server.logging.properties`, which is located in the folder `WEB-INF/classes`. If you encounter any errors that you cannot explain, consult the content of the log file.

If you are following this manual to perform a fresh installation, all the software has now been installed. What remains, is some configuration, as described in Section 2.7, “Configuring the security settings for user accounts” and Section 4.1, “Starting IUCLID 5”.

2.7. Configuring the security settings for user accounts

IUCLID 5 has features designed to control the level of security of authentication of user accounts. The level of security can be tailored to that required for the particular instance of IUCLID 5. For example, when setting passwords for their user accounts, users can be forced to enter values that have a minimum strength. The values of the parameters that determine the level of security are defined in two settings files, `server.properties` and `client.properties`, both of which are located in the folder `webapps/i5server/WEB-INF/classes/`. Changes to values take effect on restarting the **server** software of IUCLID 5. The security features are described below, grouped together by settings file.

2.7.1. User account security settings defined in `client.properties`

The settings are shown below as they appear in the settings file that is supplied with the installation of IUCLID 5. The values are shown set to the hard-coded defaults. If a line is commented out, the default value is used. A value of zero (0) disables a feature.

```
# The minimum length for a new password
password.min.length=6
# The minimum number of character sets used in the password
password.min.charsets=2
# If a secure question system is enabled
password.use.secure.question=true
```

2.7.1.1. Minimum password length

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least this number of characters. If an attempt is made to create a password with fewer characters, an informative error message is given and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum length of passwords is increased, users can still log in using existing passwords, even if they are now considered to be too short. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.7.1.2. Minimum number of character sets in passwords

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least one character from all the character sets. The value is an integer from 1 to 4. A value of 1 means only character set 1, a value of 2 means both character sets 1 and 2, etc. The four character sets are: 1 = a lowercase letter [a-z], 2 = an uppercase letter [A-Z], 3 = a digit [0-9], 4 = a non-alphanumeric symbol [!@#$%^&*-_=+].

For example, if the value is 3, a password of "AdkbScfw" is rejected for being too weak, but "AdkbSc37" is accepted because it contains at least one character from sets 1, 2 and 3.

If an attempt is made to create a password that does not comply, an informative error message is given, and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum number of character sets allowed within passwords is increased, users can still log in using existing passwords, even if they are now considered to contain too few character sets. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.7.1.3. Security question

This feature is designed to allow an alternative method of user authentication to the user name/password combination. It can help to reduce the resources required for user management by preventing account blocking due to forgotten passwords. Each user can define their own security question and a secret answer. This is done from the graphical user interface of the client, after the user has logged in. A user can log in by answering their question correctly, instead of supplying the password. The question is answered via a link on the log in page, Forgot your password?. The feature is turned on or off for the whole instance of IUCLID 5 using a value of `true` or `false`.

2.7.2. User account security settings defined in `server.properties`

The settings are shown below as they appear in the settings file that is supplied with the installation of IUCLID 5. The values are shown set to the hard-coded defaults. If a line is commented out, the default value is used. A value of zero (0) disables a feature. A suspended account can be un-suspended by a user with user-management rights.

```
# Account expiry in days. A value of zero (0) disables the feature
account.expiry=180
# Password expiry in days. Zero (0) disables the feature.
password.expiry=90
# Max number of attempts before the account is disabled. Zero (0) disables the feature.
max.failed.login.attempts=3
# Max number of attempts to answer the reset question.
max.failed.answer.attempts=3
```

2.7.2.1. Account expiry period

This feature is used to automatically suspend an account that has not been used for a long time. If the period between two successive successful log in attempts exceeds the value, the account is suspended.

2.7.2.2. Password expiry period

This feature is used to prevent users from using the same password for long periods. It defines the life-span of a password. After the password has been in use for the period, the user is prompted to change the password when they next log in. The period is counted from the time of first logging in to the account, then after that, from the time of changing the password.

2.7.2.3. Maximum number of attempts to log in

This feature is used to prevent the combination of user name and password from being obtained by trial and error. The value is the maximum number of successive unsuccessful attempts there can be to log in to an account before it is suspended.

2.7.2.4. Maximum number of attempts to answer the security question

This feature is used to prevent the security question from being answered by trial and error. The value is the maximum number of successive unsuccessful attempts there can be to answer the security question before the account is suspended.

Chapter 3. Upgrade

This document describes the update process from only IUCLID 5.3.x. The version can be seen from within the interface of IUCLID 5. To see the version, start IUCLID 5, log-in, then click *Help* and select *About*. To upgrade from IUCLID 5.2 or earlier to IUCLID 5.4, first upgrade to IUCLID 5.3.2, then follow the steps in this chapter. The software packages and instructions required to upgrade to IUCLID 5.3.2 are available on the IUCLID web site.

Before starting the upgrade, it is important to back-up the database. Use the built-in back-up functionality of IUCLID, and/or the back-up functionality of the database. Making only a copy of the file system on which IUCLID is installed is not recommended as a means of backing-up.

Warning

The built-in back-up functionality of IUCLID 5.3.1 is known to output files in which the user accounts cannot be used on restore. If you wish to use the built-in back-up functionality on data in an installation of IUCLID 5.3.1, first upgrade it to IUCLID 5.3.2. The built-in back-up functionality in IUCLID 5.3.2 does not suffer from this problem.

The migration process changes the IUCLID database such that it can no longer be used with previous versions of the IUCLID application. Therefore, if you would like to be able to continue to use a database with the previous version of IUCLID, do not run the migration tool on that particular database. Either perform a fresh installation of the new version of IUCLID and transfer the data across to it using Back-up/Restore, or perform the upgrade and migration on a duplicate of the old database. If two versions of IUCLID are to be run on the same computer, appropriate database settings must be used to avoid conflicts. Do not run two distributed versions of IUCLID at the same time on the same computer.

3.1. Upgrade and migration of data from IUCLID 5.3.x to IUCLID 5.4

There are various different ways to manage a Tomcat web application server, as referred to in the section of this manual Deployment of IUCLID 5. The following instructions are intended to give a representative example of how the IUCLID 5 software can be upgraded and the data migrated from IUCLID 5.3.x to 5.4.

1. Back-up the database. Use the built-in back-up functionality of IUCLID 5, and/or the back-up function of the database software, for example PostgreSQL. The built-in backup feature is accessible by only the user `SuperUser`, from the menu File / Administrative tools / Backup.
2. Close all clients for IUCLID 5.
3. Use the application Tomcat Manager to stop the IUCLID 5.3.x web application.
4. Copy the configuration file for IUCLID 5.3.x, `server.properties`, into a backup folder. Note that the plugins for IUCLID 5.3.x are not compatible with IUCLID 5.4. Therefore, they must *not* be copied over to the new installation.

   For example:

   copy `%TOMCAT%\webapps\i5server\WEB-INF\classes\server.properties`

   to

   `e:\backup\server.properties`
5. Use the application Tomcat Manager to undeploy the IUCLID 5.3.x web application.
6. Use the application Tomcat Manager to deploy the IUCLID 5.4 web application.

7. Stop Tomcat.

8. Copy any values that are specific to your system from the previous version of the file `server.properties` to that supplied with the new version of IUCLID 5. Ensure that the new values for the database connection are those for the database of the system to be upgraded.

Tip

IUCLID 5.3.2 was the first version of IUCLID 5 for which the file `client.properties` contained values that might need to be changed. The file is in the same folder as the file `server.properties`. The settings are for the security features for user accounts. See Section 2.7, “Configuring the security settings for user accounts” for more details.

9. Note that if the Oracle database is used, the file `server.properties` must contain the following entry. Add it or edit the existing entry if required.

```
hibernate.connection.driver_class=oracle.jdbc.OracleDriver
```

10. If the database is an Oracle database, please note that the driver for Java is no longer supplied with the IUCLID 5 installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Java 1.6 and Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`.

11. The database and all the data it contains are migrated from the previous to the new version by running IUCLID 5.4 in update mode, only once. IUCLID 5.4 is instructed to start in update mode by the line shown below in the file `server.properties`.

```
database.update.startup=true
```

The line is supplied, although commented out, in the file `server.properties` in the installation package for IUCLID 5.4. To run in update mode, the line must be either uncommented or added as shown above.

12. To begin the migration, start Tomcat. This automatically starts the new version of the IUCLID 5 web application.

Dependent on the quantity of data in the database, and the system resources available, the migration process can take from minutes to many hours. It is essential that the migration process is not interrupted. The progress of the migration can be monitored from the log files `i5server.log` and `iuclidMT.log` . The default location of these files is on the top level directory of the Tomcat installation. The file `i5server.log` contains statements about the start and end of the migration process. The file `iuclidMT.log` contains full details. If you need to know what happened during the migration process, check those files first.. At the start of the process the following entry is shown:

```
integration.database.scripts.ScriptUtils - Checking Database Status...
(eu/eca/iuclid/server/integration/database/scripts/migrate_schemav50_
to_schemav51.xml)
integration.database.scripts.ScriptUtils - Upgrading table
integration.database.scripts.ScriptUtils -

************************************

Database changes are being applied now.
This process might, depending on the size of your database, take some time
(several minutes to perhaps hours). Please do NOT shutdown the system as this
might result in an inconsistent database state.
```

As the migration proceeds, details of which data are being migrated are written to `iuclidMT.log`. The end of a successful migration is indicated by the following entry:

```
integration.database.scripts.ScriptUtils - Database update successfully finished.
integration.database.scripts.ScriptUtils - Checking Database Status...
(eu/eca/iuclid/server/integration/database/scripts/
migrate_schemav51_patch.xml)
integration.database.scripts.ScriptUtils - Upgrading table
integration.database.scripts.ScriptUtils - Database is up to date.
```

If the migration is interrupted, or fails, for whatever reason, the database must be restored from the back-up and the migration started again.

13. When the migration finishes successfully, stop the new version of the IUCLID 5 web application by stopping Tomcat.

14. Set IUCLID 5 to start *not* in its update mode by commenting out the line edited previously:

```
#database.update.startup=true
```

15. Start Tomcat.

16. Run the IUCLID 5 client in the same way as before the upgrade. The initialisation process is not required. All of the data that was present before the upgrade should be present in the new system. Therefore, it should be possible to log in to any of the user accounts that were present prior to the upgrade.

17. Log in to the IUCLID 5 client as one of the users that was present before the upgrade.

18. Confirm that the version of IUCLID 5 is the new, expected version. This can be seen from the menu Help / About.

19. Confirm that the data from the previous version has been successfully migrated to the new version.

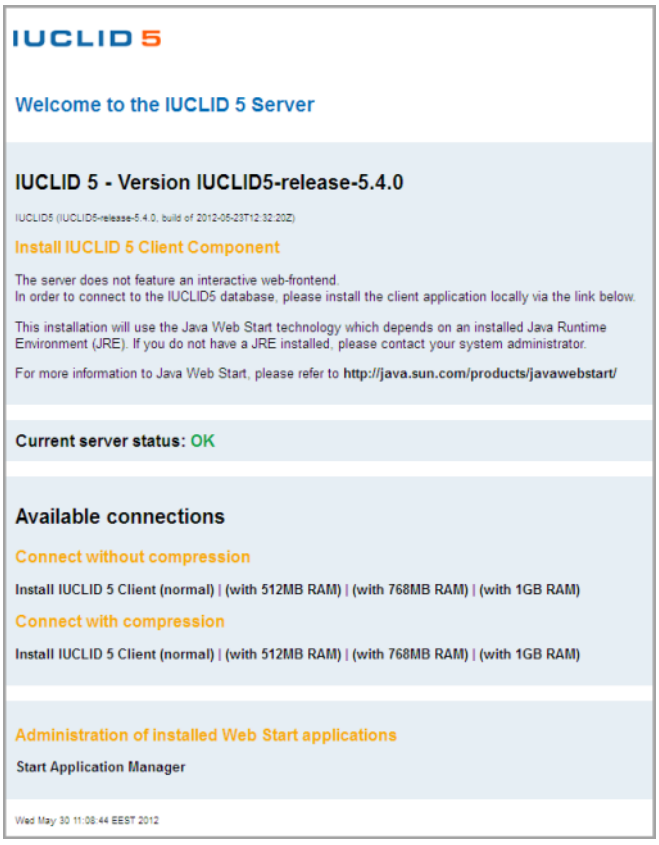
Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a back-up that was made using the built-in back-up function of IUCLID. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from back-up, make sure that the back-up files are accessible from the system on which IUCLID will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Connect to the application with a browser by entering the address *http://<address of your server>:8080/i5server*. An example of the page displayed is shown below.

Figure 4.1. Example default page for Java Web Start of IUCLID 5


IUCLID 5
Welcome to the IUCLID 5 Server
IUCLID 5 - Version IUCLID5-release-5.4.0
IUCLID5 (IUCLID5-release-5.4.0, build of 2012-05-23T12:32:20Z)
Install IUCLID 5 Client Component
The server does not feature an interactive web-frontend.
In order to connect to the IUCLID5 database, please install the client application locally via the link below.
This installation will use the Java Web Start technology which depends on an installed Java Runtime Environment (JRE). If you do not have a JRE installed, please contact your system administrator.
For more information to Java Web Start, please refer to http://java.sun.com/products/javawebstart/
Current server status: OK
Available connections
Connect without compression
Install IUCLID 5 Client (normal) | (with 512MB RAM) | (with 768MB RAM) | (with 1GB RAM)
Connect with compression
Install IUCLID 5 Client (normal) | (with 512MB RAM) | (with 768MB RAM) | (with 1GB RAM)
Administration of installed Web Start applications
Start Application Manager
Wed May 30 11:08:44 EEST 2012

The page shown above page contains links that use Java Web Start technology to start a client that connects to the IUCLID server and displays IUCLID 5's graphical user interface (GUI) on the client machine. In the example shown above, the link under the text *IUCLID 5 Client (with 1GB RAM)* has already been followed. The difference between the links in the above page is that each link passes different parameters to the IUCLID 5 server. The options included are for varying amounts of memory to be allocated to IUCLID 5 and for different types of data compression to be employed in the connection to the server. If IUCLID 5 runs slower than you would like and you have the available memory, select a link for a larger amount of RAM. The client can be run directly from a browser or by first downloading

a file from one of the links and running that. Depending on your browser settings, when you click on one of the links above you will see either a dialogue box, or IUCLID 5 will run and you will see the login page. The browser dialogue asks whether you would like to save a file or run it straight away. The choice is yours. A convenient way to access IUCLID 5 is to download one of the files from the default page, save it to the desktop of your local machine used to access IUCLID 5 and give it the IUCLID 5 icon that comes with the installation. Double clicking on the icon then launches the IUCLID 5 GUI. Once you see the login page, you are ready to go through the *First steps* wizard, as described in the next section.

4.2. First steps wizard

When you start IUCLID 5 for the first time, the *First steps* wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 End-user Manual.

Important

This wizard allows a single user account to be created, per run. This user is in addition to the *SuperUser* account that comes with the installation. It is essential to have at least one user account in addition to *SuperUser* because *SuperUser* should be used only for the special tasks that only it can carry out. See the IUCLID 5 End-user Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 End-user Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 End-user Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the *SuperUser*. This is done from the file menu within IUCLID 5 **Administrative tools** / **Initialise**.

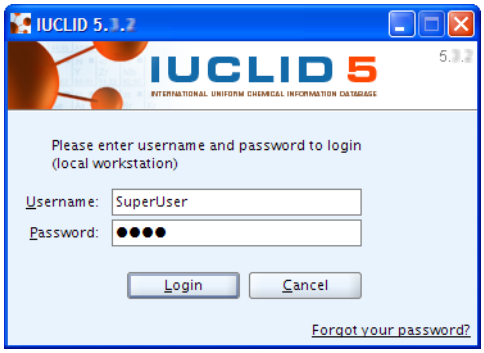
When starting the IUCLID 5 for the first time, the only user available is an administrator named *SuperUser*. Log in as *SuperUser* by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

Password: root

Note

Do not click on the link **Forgot your password?** if the *First steps* wizard is being run for the first time on this database. This feature can work only after the wizard has been completed. The use of the feature **Forgot your password?** is explained later in this wizard, at step 3.



The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

Figure 4.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the **Next** button.

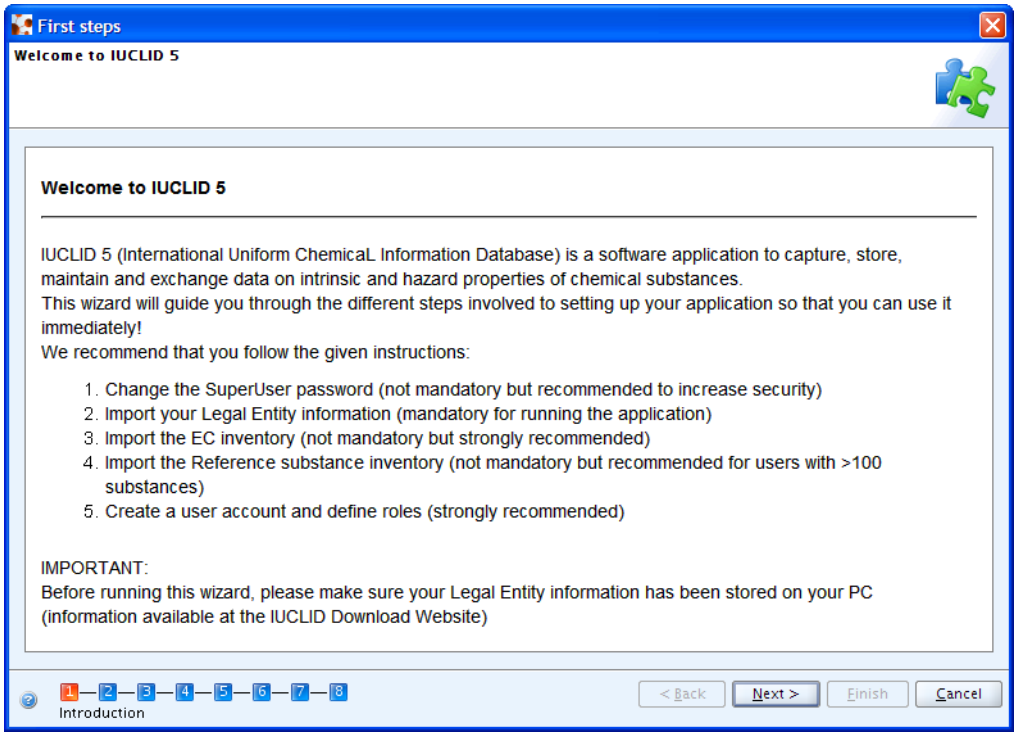

First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately!
We recommend that you follow the given instructions:
1. Change the SuperUser password (not mandatory but recommended to increase security)
2. Import your Legal Entity information (mandatory for running the application)
3. Import the EC inventory (not mandatory but strongly recommended)
4. Import the Reference substance inventory (not mandatory but recommended for users with >100 substances)
5. Create a user account and define roles (strongly recommended)
IMPORTANT:
Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
1 2 3 4 5 6 7 8
Introduction
< Back
Next >
Finish
Cancel

Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button `New Installation`as shown below and continue to the next step.

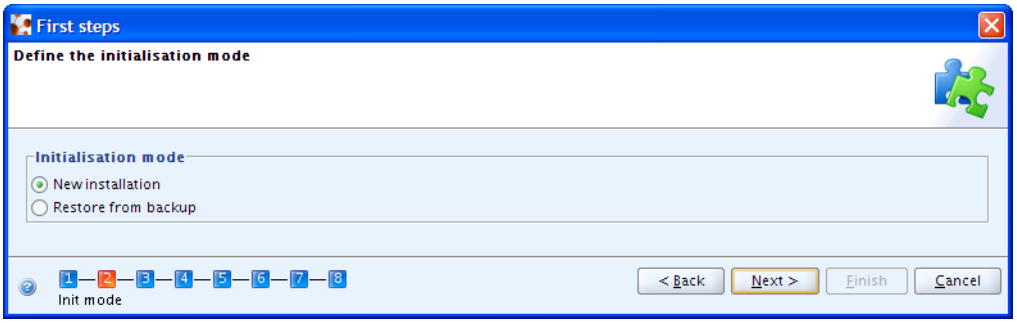
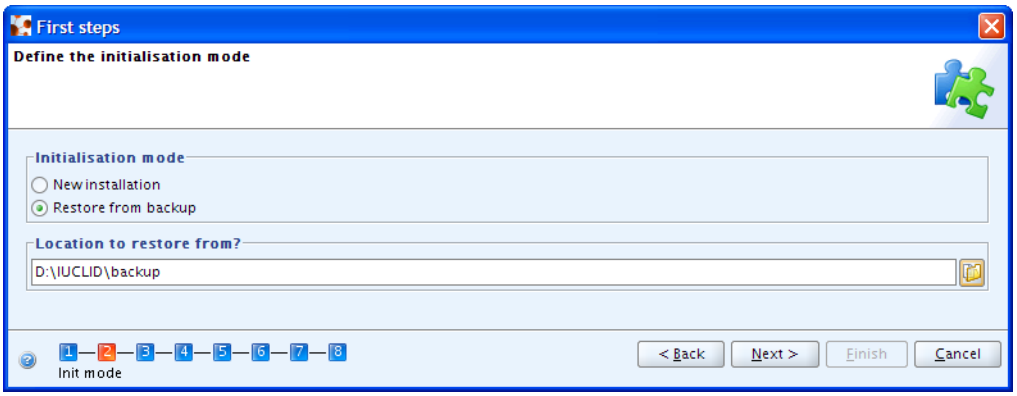


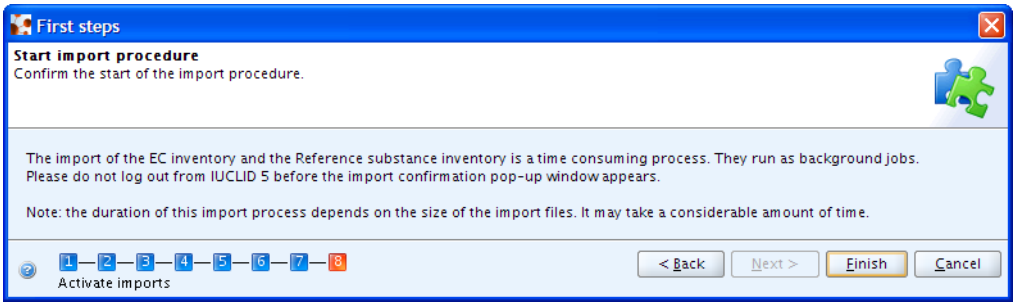
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button `Restore from backup` then enter the directory containing the backup files as shown in the example below.



Click **Next**. The wizard jumps to its last step, where the importation of data is started, as shown below.

Figure 4.5. Restoration from a back-up - Step 8 - Activate imports


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

The import may take some time. Click *Finish*. When the restoration is complete, the following screen is shown.

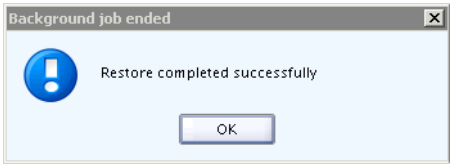
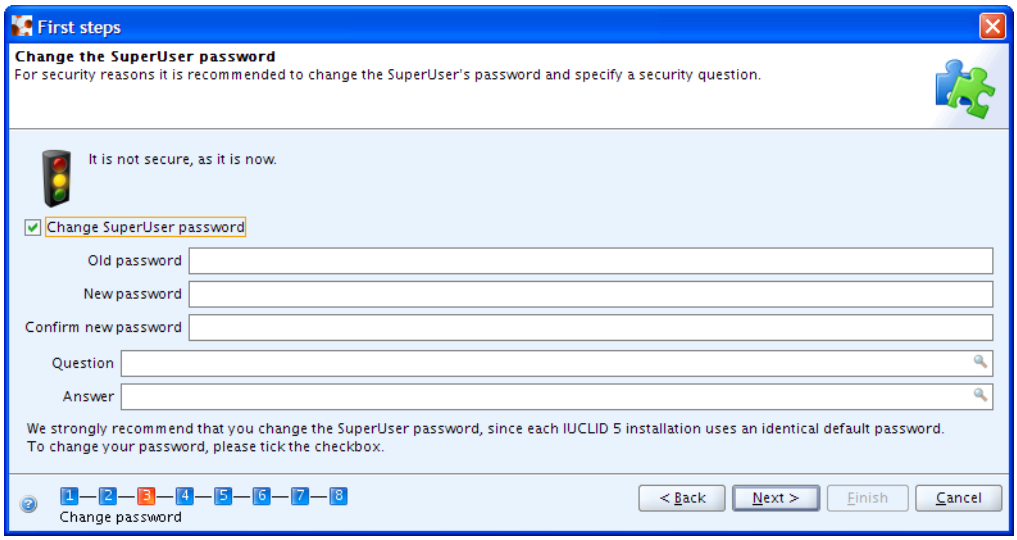


Figure 4.6. Step 3 of the First steps wizard - Change password

If the password for *SuperUser* has never been changed from its default value of *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box `Change SuperUser password` , enter the current password, and then the new password, and then the new password again.

To proceed, click the button **Next**.


First steps
Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password and specify a security question.
It is not secure, as it is now.
Change SuperUser password
Old password
New password
Confirm new password
Question
Answer
We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.
1 2 3 4 5 6 7 8
Change password
< Back
Next >
Finish
Cancel

Tip

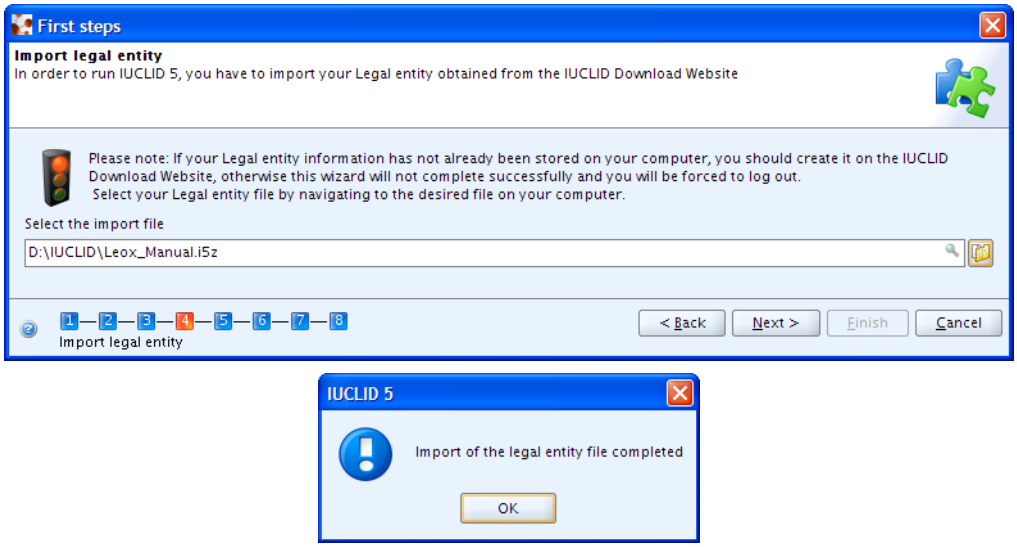
IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

Tip

IUCLID 5 has a feature that allows a user to log in by answering a security question, instead of providing the password for the account. Users define their own questions and answers from within their own accounts. However, the SuperUser is a special case, because the question and answer can be defined before logging in for the first time. The question and answer are entered into the fields shown above in step 3 of the wizard. To use the feature to log in, a user clicks on the link **Forgot your password?** which is situated at the bottom right of the login page.

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 End-user Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field Select the import file. Click the **Next** button. The Legal entity is imported immediately.


First steps
Import legal entity
In order to run IUCLID 5, you have to import your Legal entity obtained from the IUCLID Download Website
Please note: If your Legal entity information has not already been stored on your computer, you should create it on the IUCLID Download Website, otherwise this wizard will not complete successfully and you will be forced to log out.
Select your Legal entity file by navigating to the desired file on your computer.
Select the import file
D:\IUCLID\Leox_Manual.i5z
1 2 3 4 5 6 7 8
Import legal entity
< Back
Next >
Finish
Cancel
IUCLID 5
Import of the legal entity file completed
OK

Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

Figure 4.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 End-user Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

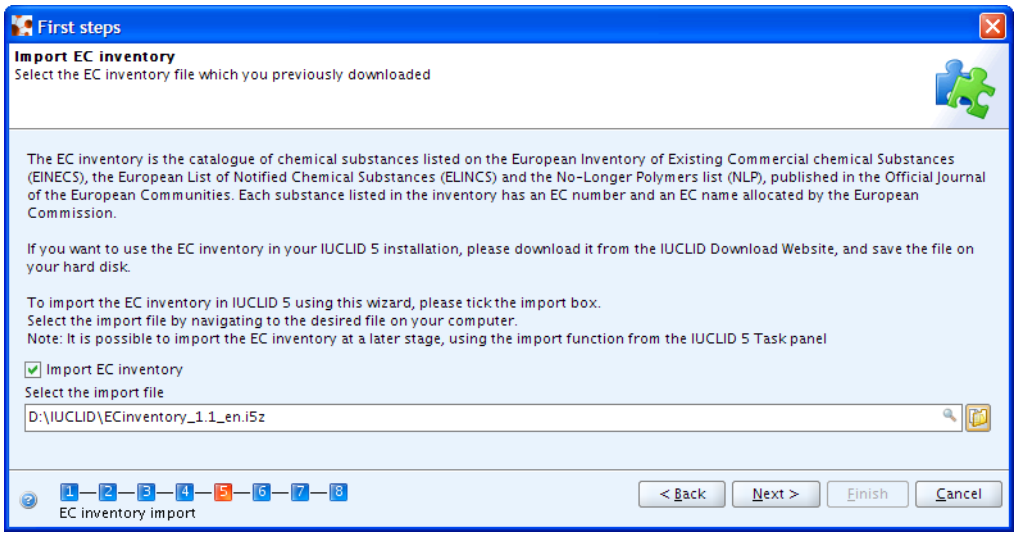
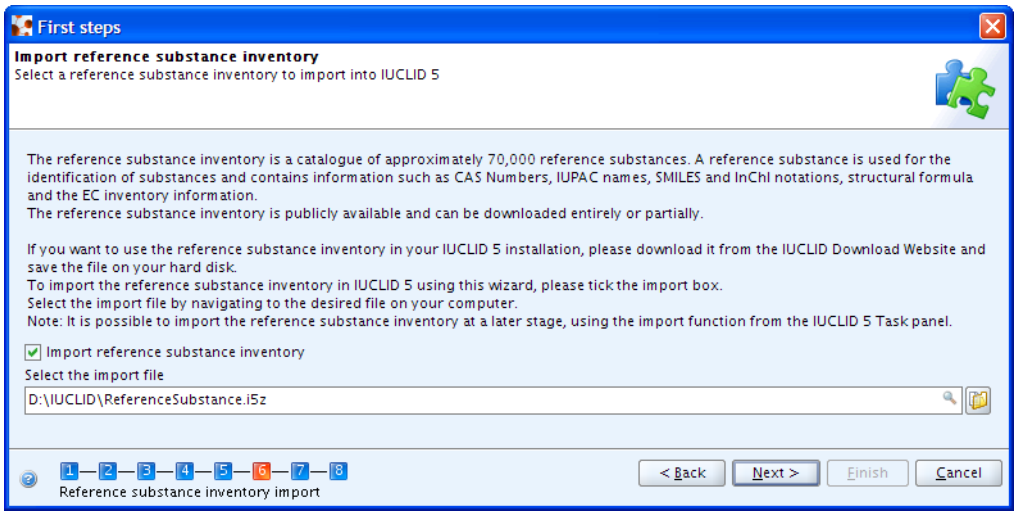

First steps
Import EC inventory
Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journal of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
Import EC inventory
Select the import file
D:\IUCLID\ECinventory_1.1_en.i5z
1 2 3 4 5 6 7 8
EC inventory import
< Back
Next >
Finish
Cancel

Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 End-user Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a long time. The import of the Reference substance inventory itself can take **up to several hours**.

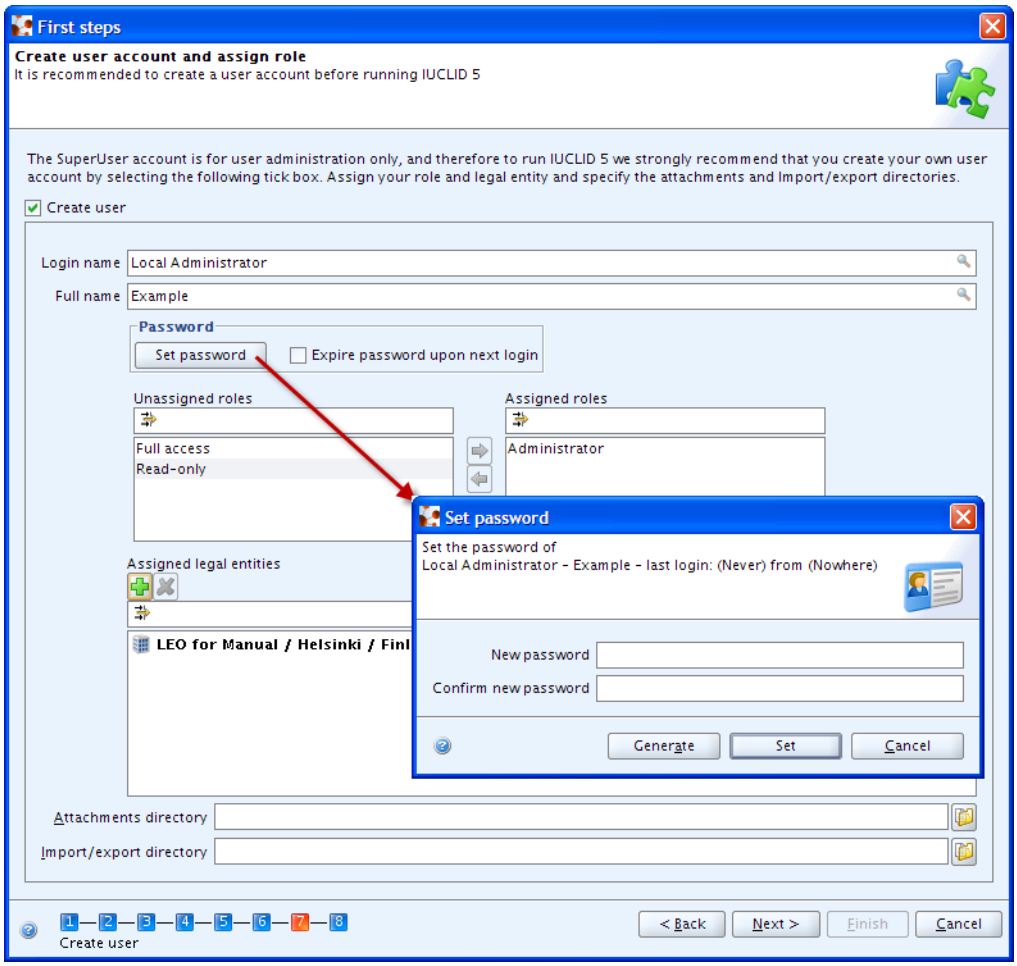

First steps
Import reference substance inventory
Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information.
The reference substance inventory is publicly available and can be downloaded entirely or partially.
If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk.
To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel.
Import reference substance inventory
Select the import file
D:\IUCLID\ReferenceSubstance.i5z
1 2 3 4 5 6 7 8
Reference substance inventory import
< Back
Next >
Finish
Cancel

Tip

Time and IT resources can be saved by importing into IUCLID only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set,* a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.


First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directories.
Create user
Login name
Local Administrator
Full name
Example
Password
Set password
Expire password upon next login
Unassigned roles
Full access
Read-only
Assigned roles
Administrator
Assigned legal entities
LEO for Manual / Helsinki / Finl
Set password
Set the password of
Local Administrator - Example - last login: (Never) from (Nowhere)
New password
Confirm new password
Generate
Set
Cancel
Attachments directory
Import/export directory
1 2 3 4 5 6 7 8
Create user
< Back
Next >
Finish
Cancel

- Select the checkbox `Create user`.

  Fill in all the fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions. In a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default.

- Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Click *Set password* to define a password.

Tip

IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file

within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

Tip

If you want a use-once password that is reasonably hard to guess and that definitely conforms to the password policy, you can let IUCLID 5 make one for you, by clicking on the button *Generate*. It will be displayed in a new window for you to make a record of it. On closing that window it will be automatically entered into the fields *New password* and *Confirm new password*.

- Ticking the box *Expire password upon next login* forces whoever logs in to the account first to set their own password.

- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default).

Tip

It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 End-user Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.

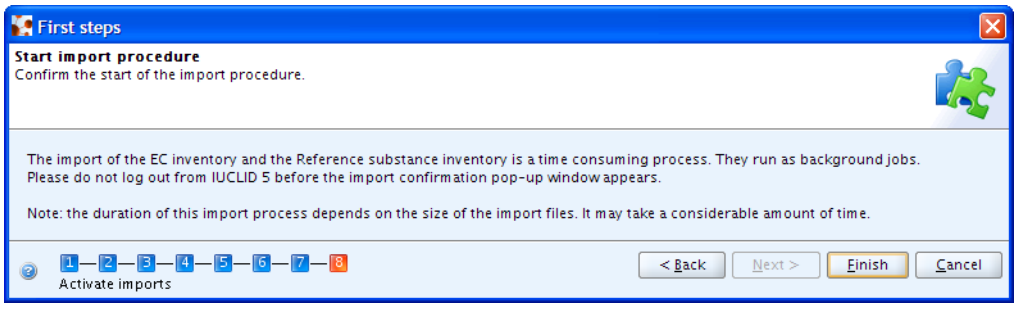
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 End-user Manual.

- Click the **Next** button

Figure 4.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

4.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 End-user Manual. Individual users can connect to the IUCLID 5 server using Java Web Start technology, as described in Section 4.1, “Starting IUCLID 5”. A convenient way to achieve that is for users to save onto their desktop, one of the files downloaded from the default Java Web Start page. The user would launch IUCLID 5 by simply double-clicking on the icon on his or her desktop. Alternatively, the users could be supplied with the URL *http://<address of your server>:8080/i5server* and instructions on which link to use.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID is a manual process. IUCLID can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.